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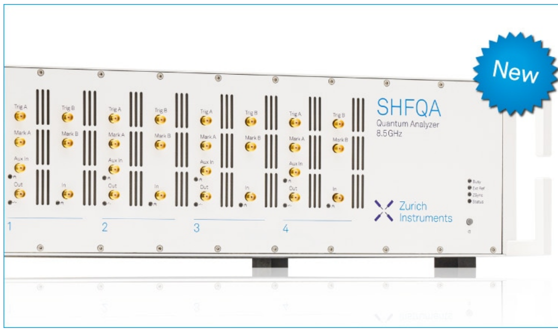

Mathematical modelling of the spatial network of bone implants obtained by 3D-prototyping

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Abstract. In this paper, the mathematical model suitable for bone implants 3D-prototyping is proposed. The composite material with the spatial configuration of reinforcement with matrix of hydroxyapatite and titanium alloys fibers is considered. An octahedral cell is chosen as an elementary volume. The distribution of reinforcing fibers is described by textural parameters. Textural parameters are integrated characteristics that summarize information on the direction of reinforcing fibers and their volume fractions. Textural parameters, properties of matrix and reinforcing fibers allow calculating effective physical and mechanical properties of the composite material. The impact of height and width of the octahedral reinforcement cells on textural parameters of the composite material is investigated in this work. The impact of radius of fibers is also analyzed. It is shown that the composite becomes quasi-isotropic under certain geometrical parameters of cell.

INTRODUCTION

High-porous materials are often used in the design of new types of bone implants [1–3]. This requirement is dictated by the fact that the high-porous material has a better biocompatibility compared to the non-porous material. The bone tissue cells grow into the implant pores [4]. In addition, the connected pores facilitate the delivery of body fluids to the neoformed tissue. In this respect, there is a need to provide new materials that exhibit, on the one hand, high porosity, and on the other hand, sufficiently high strength characteristics in order to use them in the high-loaded skeletal parts.

One of such materials is the composite with titanium / titanium alloy reinforcement and matrix of hydroxyapatite – the material that is chemically similar to the bone mineral.

As a result of combining the reinforcing elements and the matrix, there is formed a complex of composite properties, not only determined by the initial characteristics of components, but also including properties that are not found in isolated components [5]. Directional properties are included in the most important advantages of composite materials; they allow creating structural elements with predetermined properties that meet the work conditions. The mechanical characteristics of composite materials that are conditioned upon the fiber layout can vary over a wide range. In addition to creating a variety of geometric shapes, manufacturing of composite structures requires the definition of a rational material structure – fiber orientation angles, their count and interlacing, type of reinforcing elements, their proportion in the composition and other parameters.

Numerical approaches are abundant among the methods for determining effective properties of composites. There are several methods for calculating effective properties: the calculation of composite material properties produced by its components properties [6], the allocation of periodic structures in the composite structure with a further solution of boundary value problems [7–9], the asymptotic averaging method [10–11]. The basis of these methods is either an approximate analysis of physical fields, or calculation of physical and mechanical

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characteristics of the material at the level of elementary volumes, followed by the connection. The analytical determination of effective properties of composite material requires information about properties of fibers and matrix. In addition, it is necessary to assess quantitatively the geometry of the composite. In this work, textural parameters are used to describe the reinforcing fibers direction and their volume fractions [12].

AIM

The aim of this study is to analyze the impact of height and width of cells and radius of the reinforcing fibers on textural parameters of the composite material. The investigated material is the composite with the spatial configuration of reinforcement. The reinforcement is defined by the octahedral array of cells composed of cylindrical fibers.

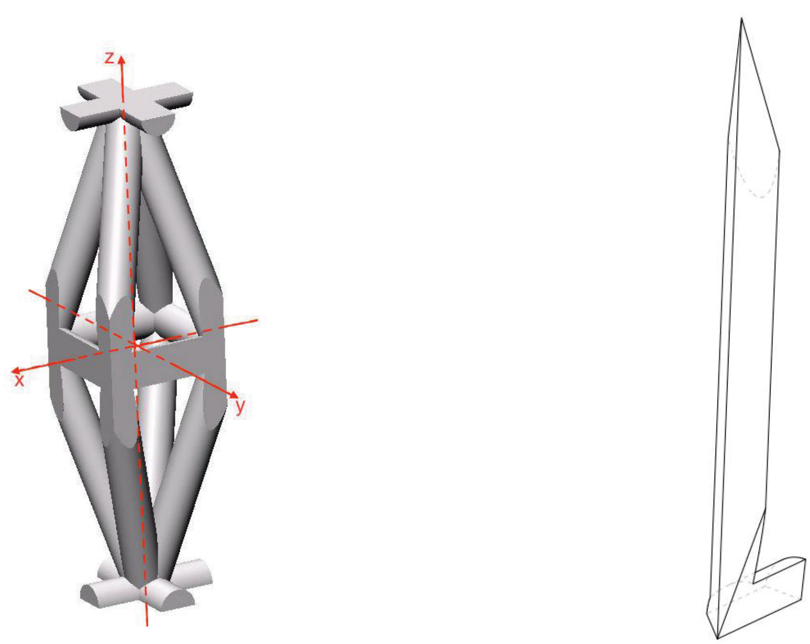
MATHEMATICAL MODEL

The figure shown in Fig. 1 (a) is chosen as an elementary cell. We introduce the coordinate system, whose axes coincide with the axes of symmetry of the octahedron, and the coordinate origin coincides with a center of symmetry. The directions of OX and OY axes coincide with the directions of the octahedron edges lying at its base. OZ axis connects two opposite octahedron vertices that do not belong to its base.

The model of reinforcement of the considered composite material is obtained by the translation of elementary cells along the coordinate axes. The effective mechanical properties of the material and the proportional volume fractions of fibers in the whole composite and in the elementary cell are the same.

Because of the symmetry of the elementary cell, we consider the part of it: its form is shown in Fig. 1 (b); next, it is partitioned into an inclined volume (Fig. 2 (a)) and a horizontal volume (Fig 2. (b)).

To calculate the volumes of parts, the planes limiting these volumes are set. The local coordinate system is introduced in the inclined and horizontal volumes. In the inclined volume, the direction of OZ axis coincides with the direction of the lateral edge of the octahedral elementary cell. OY axis lies in the diagonal symmetry plane of the octahedron. In the horizontal volume, OZ axis is directed along the octahedron edge lying at its base. OY axis lies in the horizontal symmetry plane of the octahedron.



(a) (b)

FIGURE 1. (a) elementary reinforcement cell; (b) part of the elementary cell partitioned using its symmetry

(a) (b)

FIGURE 2. (a) inclined volume of the cell part, (b) horizontal volume of the cell part

Matrices of the transition to local coordinate systems of inclined and horizontal parts:

$$\begin{pmatrix} \frac{\sqrt{a^2+2h^2}}{\sqrt{2a^2+4h^2}} & \frac{\sqrt{a^2+2h^2}}{\sqrt{2a^2+4h^2}} & 0 \\ \frac{-\sqrt{2}h}{\sqrt{2a^2+4h^2}} & \frac{\sqrt{2}h}{\sqrt{2a^2+4h^2}} & \frac{-\sqrt{2}a}{\sqrt{2a^2+4h^2}} \\ \frac{-a}{\sqrt{2a^2+4h^2}} & \frac{a}{\sqrt{2a^2+4h^2}} & \frac{2h}{\sqrt{2a^2+4h^2}} \end{pmatrix}, \quad \begin{pmatrix} 0 & 0 & 1 \\ -1 & 0 & 0 \\ 0 & -1 & 0 \end{pmatrix}, \tag{1}$$

where h is the half of the octahedron height, and a is the width of the octahedron base.

As a result of the forth integration, the volume of the inclined part (V_n) and the volume of the horizontal part (V_l) are obtained. The total volume of fibers in the elementary cell:

$$V = 32(V_l + V_n). \tag{2}$$

The porosity of the material is determined by the ratio:

$$\Pi = 1 - \frac{V}{2*h*a^2}. \tag{3}$$

TEXTURAL PARAMETERS

Textural parameters are introduced to calculate the macroscopic characteristics of the composite material [12]. For the composite with fibers that are distributed in several discrete directions, textural parameters are determined by the expressions:

$$\begin{gathered} \Delta_1 = \sum_k p_k cos^2\phi_k sin^2\gamma_k,\ \Delta_2 = \sum_k p_k sin^2\phi_k sin^2\gamma_k,\ \Delta_3 = \sum_k p_k cos^2\gamma_k, \\ \Delta_4 = \sum_k p_k cos^4\phi_k sin^4\gamma_k,\ \Delta_5 = \sum_k p_k sin^4\phi_k sin^4\gamma_k,\ \Delta_6 = \sum_k p_k cos^4\gamma_k, \end{gathered} \tag{4}$$

where p_k is the volume fraction of fibers with a certain orientation, ϕ_k and γ_k are the spherical angles that set the position of a certain way oriented fiber in the coordinate axes associated with the composite. Textural parameters for the bone implant:

$$\Delta_1 = \Delta_2 = \frac{16}{V} * \left(\frac{V_n a^2}{(2h^2+a^2)} + V_l\right), \quad \Delta_3 = \frac{64}{V} * \frac{V_n h^2}{(2h^2+a^2)}, \tag{5}$$

$$\Delta_4 = \Delta_5 = \frac{8}{V} * \left(\frac{V_n a^4}{(4h^4+4a^2h^2+a^4)} + 2V_l\right), \quad \Delta_6 = \frac{128}{V} * \frac{V_n h^4}{(4h^4+4a^2h^2+a^4)}. \tag{6}$$

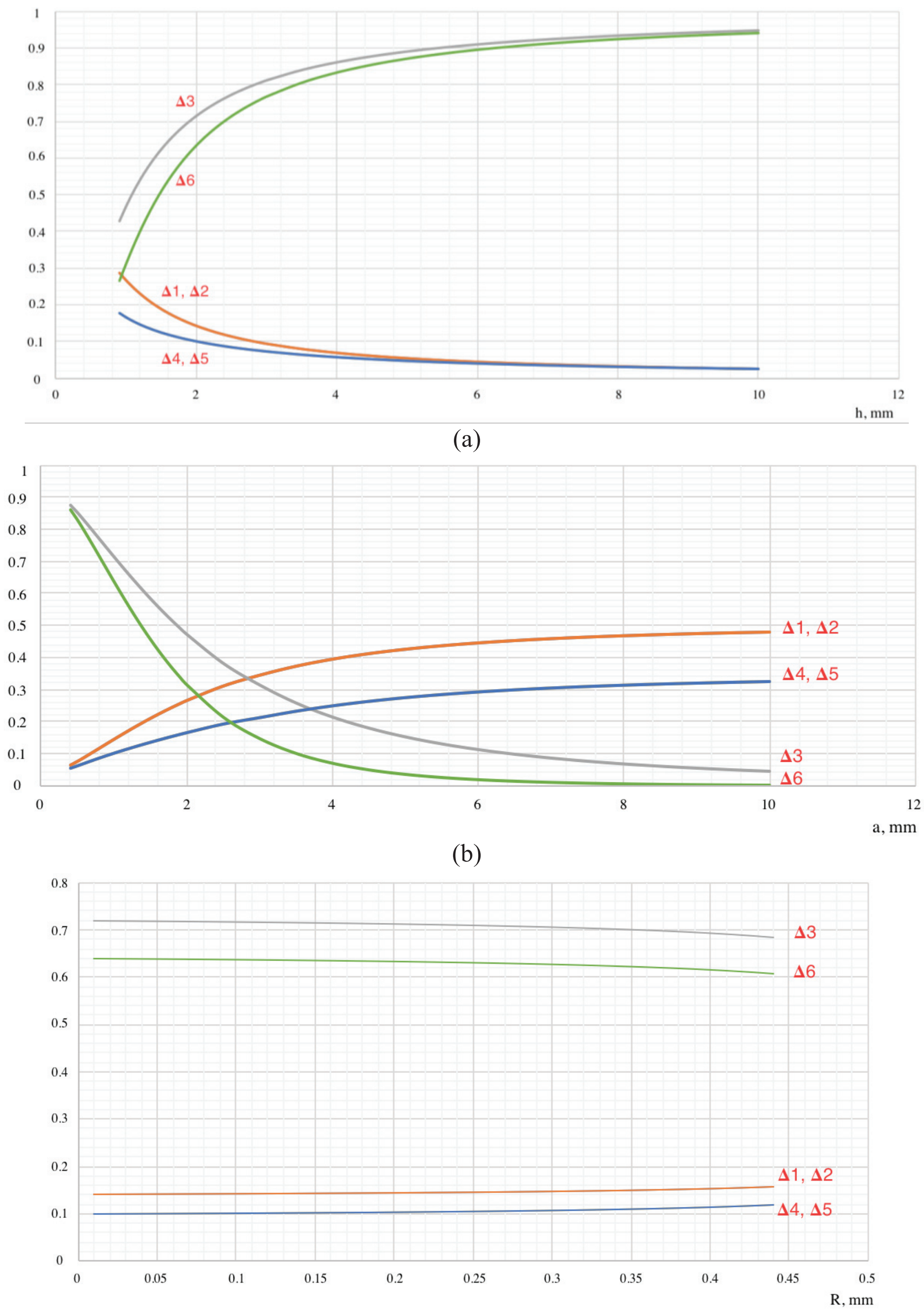


FIGURE 3. Investigating the impact of cell height, cell width and fibers radius on textural parameters. (a) Impact of height on textural parameters. (b) Impact of cell width on textural parameters. (c) Impact of fibers radius on textural.

THE IMPACT OF GEOMETRIC PARAMETERS OF CELL AND FIBERS RADIUS ON TEXTURAL PARAMETERS

To automate the calculation of texture parameters, the macro was developed, that allows obtaining the parameter values from the known values of width and height of octahedral cell and radius of reinforcing fibers.

In the course of the numerical experiment, we assigned constant values for two of three concerned parameters; the value of the third parameter was varied. The following values were selected as the constant values: cell height – 2 mm, cell width – 1 mm, fibers radius – 0,15 mm. The results of investigating the impact of cell height on textural parameters are shown in Fig. 3 (a), the impact of cell width – in Fig. 3 (b), the impact of fibers radius – in the Fig.3(c). Fig. 3 (a) shows the graph of variance of textural parameters when changing the octahedral cell height. The graph shows that with increasing the cell height such parameters, as, Δ_1, Δ_2, Δ_4, Δ_5 tend to zero, and Δ_3, Δ_6 tend to unity. With increasing the cell width (Fig. 3 (b)) such parameters, as Δ_3 and Δ_6 decrease sharply while such textural parameters, as Δ_1, Δ_2, Δ_4 and Δ_5 increase. Changing the fibers radius (Fig. 3 (c)) has practically no effect on textural parameters. Fig. 3 (b) shows that textural parameters Δ_1, Δ_2, Δ_3 approach to 0.33 when the cell width is set to 2.6–2.8 mm, and Δ_4, Δ_5, Δ_6 approach to 0.2, that corresponds to the quasi-isotropic material.

CONCLUSION

Effective properties of the composite material depend on properties of matrix, fibers and fibers volume fractions. The decisive role is played by textural parameters that give information about the geometry of the composite structure. The study obtained values of textural parameters of the cellular composite. The impact of height, width of the octahedral cell, and the radius of fibers is investigated. The proposed mathematical model allows obtaining the appropriate geometric parameters of cell, as well as the radius of fibers from the known operation conditions.

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